

PNAS Supporting Information Template

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Table S1. Comparison of the fitted potential energy surfaces and ab initio benchmark electronic energy calculations

Species	CBS	CV	G3
1. Acetaldehyde	0.0	0.0	0.0
2. Vinyl alcohol	9.1	9.6	13.5
3. Hydroxyethylidene	50.8	51.2	54.0

nomenclature for the TSs refers to the numbered species in the table.

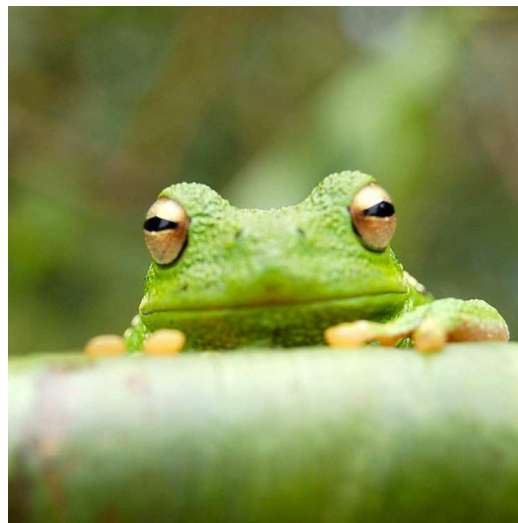


Fig. S1. Placeholder image of a frog with a long example caption to show justification setting.

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1. Varga A, Edmonds AN (2016) Multilingual extraction and editing of concept strings for the legal domain. *Advances in Computer Science: an International Journal* 5(4):18–23.
2. Olsen TE, Stensland G (1992) On optimal timing of investment when cost components are additive and follow geometric diffusions. *Journal of economic dynamics and control* 16(1):39–51.
3. Bérard P, Besson G, Gallot S (1994) Embedding riemannian manifolds by their heat kernel. *Geometric & Functional Analysis GAFA* 4(4):373–398.
4. Baklouti N, Gargouri B, Jmaïel M (2015) Towards patterns-based linguistic web service composition in *Computer Systems and Applications (AICCSA), 2015 IEEE/ACS 12th International Conference of. (IEEE)*, pp. 1–6.

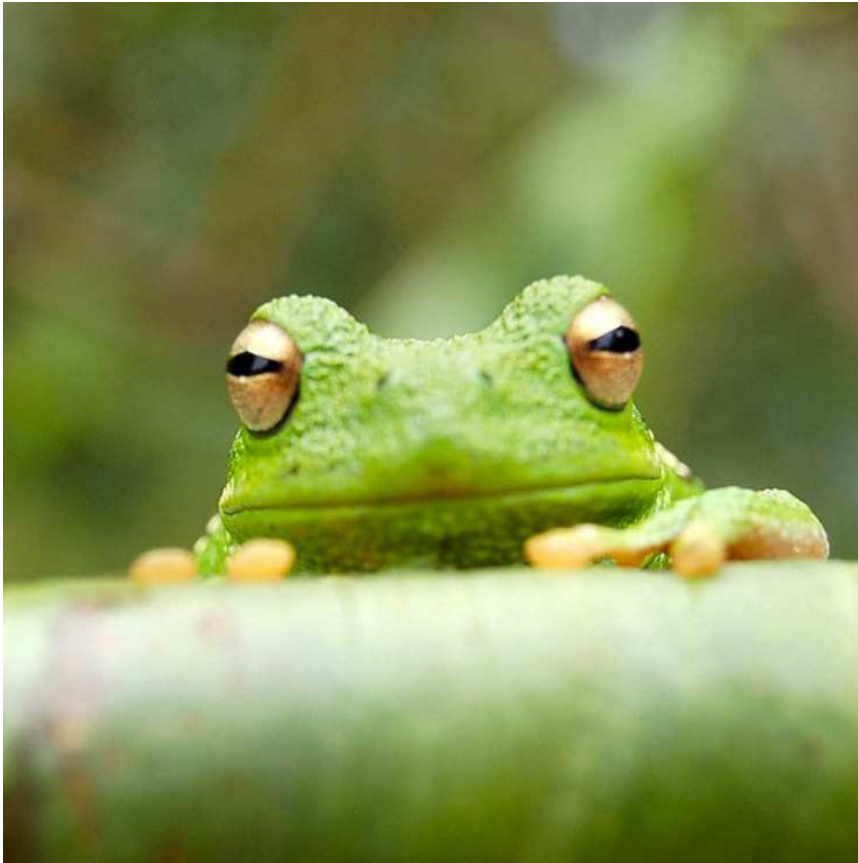


Fig. S2. This caption would be placed at the side of the figure, rather than below it.